# FAC Atomic Data in Prism Codes

Prism developed infrastructure to utilize atomic data generated by the Flexible Atomic Code (FAC) [1]. FAC is an open-source integrated software package that calculates various atomic radiative and collisional processes. The atomic structure calculation in FAC is based on the relativistic configuration interaction with independent particle basis wavefunctions. These basis wavefunctions are derived from a local central potential, which is self-consistently determined to represent electronic screening of the nuclear potential. Relativistic effects are fully taken into account using the Dirac Coulomb Hamiltonian. Higher order QED effects are included with Breit interaction in the zero-energy limit for the exchanged photon and hydrogenic approximations for self-energy and vacuum polarization effects. Continuum processes are treated in the distorted-wave (DW) approximation.

Atomic data generated by FAC are already widely used in the HEDLP research community. However, generation and utilization of the data often require substantial expertise in atomic physics. By combining advanced simulation software with open-source atomic structure calculations, Prism developed a new capability that will significantly improve modelling efforts for a wide range of plasma applications. Using FAC data is highly desirable not only because of its ability to generate atomic data for high-Z elements, but also because it can be used for supplying an alternative source of data for Prism simulation codes, a valuable feature for code validation.

FAC-generated data can be used by all simulation tools developed at Prism: radiation-hydrodynamics, imaging and spectroscopy, and EOS and opacity. EOS and opacity tables generated by the application PROPACEOS can be used not only with Prism simulation software, but also with other hydrodynamics (e.g., FLASH) and the particle-in-cell (e.g., LSP) codes.

The following algorithms were implemented:

- Full support for JJ coupling scheme in addition to existing LS coupling. FAC data are labeled according to its native convention and the level index. For FAC data, all fine-structure levels can be collapsed into configuration-averaged.
- Developed full support for atomic data generated by FAC. Selection of FAC data is implemented as an extra option in the Atomic Model Builder to specify FAC input. At present, Prism codes support only binary tables produced by FAC. This is the default option for FAC. Binary files also perform better than ASCII when read in by the simulation codes. Prism does not plan to support ASCII tables. FAC creates separate files for different types of data, e.g., energy levels are stored in one file, and oscillator strengths for transitions in another file. Thus, when selecting FAC input, the user must select corresponding files from their FAC calculation.

Three FAC output files are always required for the simulations (LTE or NLTE):

- DB_EN: energy, configuration, parity, and total angular momentum of each atomic level.

- DB_TR: oscillator strengths for radiative transitions. The file also includes the indices for lower and upper levels in each transition, transition energies, radiative decay rates, and reduced dipole matrix elements.
- DB_RR: photoionization cross sections (also has radiative recombination, not needed for LTE).

Three additional files are required for NLTE simulations:

- DB_CE: Collisional excitation cross-sections.
- DB_CI: Collisional ionization cross-sections.
- DB_AI: Autoionization rates.

Two new files can now be produced by FAC to better support integration with Prism codes. These files are optional, but if the files are not provided, some advanced modelling options may be disabled:

- DB_RP: Orbital data needed for continuum lowering and line broadening models, e.g., electron binding energies and mean radii. In FAC, all radial orbital wavefunctions are generated from a single potential, regardless of the configuration or level. So, the properties of subshells are not associated with levels (e.g., the 4s orbitals are the same whether it's in 1s2 4s1 level or in 1s1 2s1 4s1 level). Therefore, the data can be stored in a table of all subshell properties per ion without referencing energy levels.
- DB_RC: Rate coefficients for some transitions (e. g. dielectronic recombination, excitation autoionization, and resonant excitation). These rate coefficients are generally associated with some intermediate autoionizing levels, which are not explicitly included in the database prepared for Prism codes. The data in this file may be needed to make some large-scale simulations more practical.

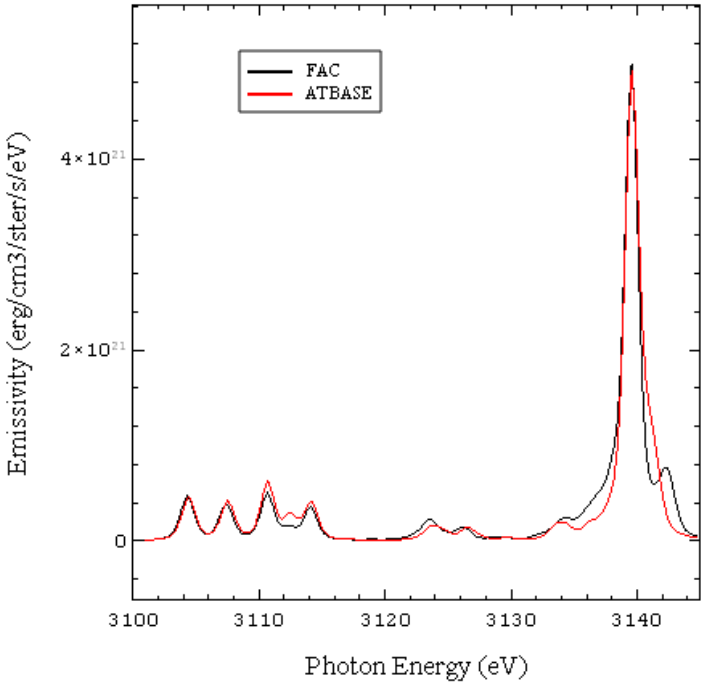
FAC stores atomic levels in order of their energy, regardless of their ionization level. Prism code requires energy levels to be grouped into ionization blocks, and energy-ordered within those blocks. Thus, an index mapping was needed for re-ordering the energy levels after reading from FAC output. In addition, FAC generally calculates atomic data for individual ions in separate processes, as the central potential used to produce the basis wavefunctions needs to be optimized for different ions. The FAC data files for different ionization stages of the same element are combined to produce a single file per process (e.g., energy levels of all ions are combined into one file, and so are those for radiative transitions, collisional excitations, ionizations, etc.).

The latest version 1.5.0 of FAC on github.com/flexible-atomic-code includes newly developed tools to prepare all the aforementioned data files needed to work with Prism software. Input scripts to streamline this workflow have also been developed and may be obtained by contacting Prism directly.

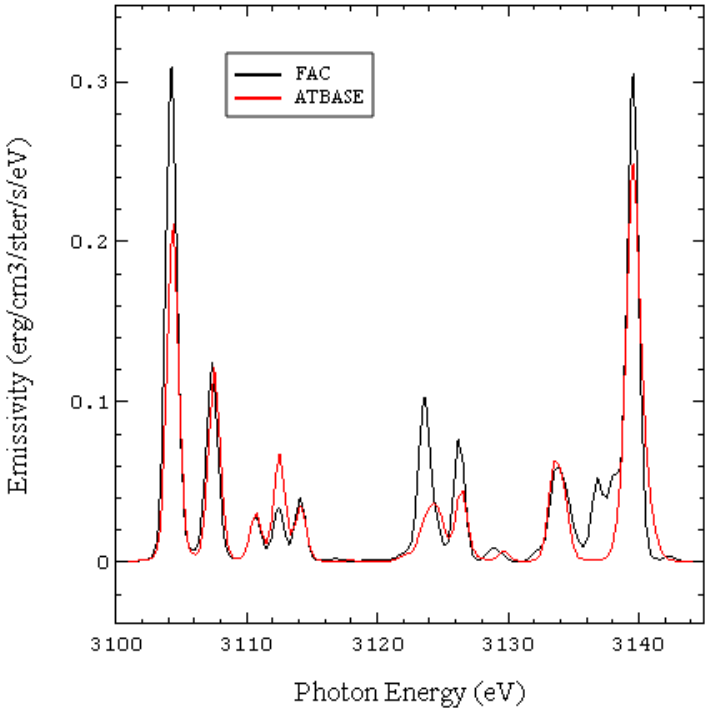
All Prism applications share the same reads for the atomic data and access the atomic databases through light-weight atomic model files (*.atm) generated by the Atomic Model Builder. Once the atomic model files are produced, the source of the underlying data (ATBASE or FAC) becomes completely transparent to the users.

Below are the results of benchmark simulations for Ar-doped DD plasma using FAC and ATBASE data. The spectral range covers Ar He alpha transition and associated Li-like satellites. The plasma is optically thin and the electron temperature is 600 eV.

At higher density (1 g/cc mass density, or ~3e23 1/cc electron number density), the spectral features in the simulation are very similar.




At lower densities (1e-11 g/cc, or 3e12 1/cc electron density), the differences in collisional cross-sections between the codes result in more significant discrepancies.



## References

1. M. F. Gu, “The flexible atomic code”, Canadian Journal of Physics**,** 86(5): 675-689 (2008)